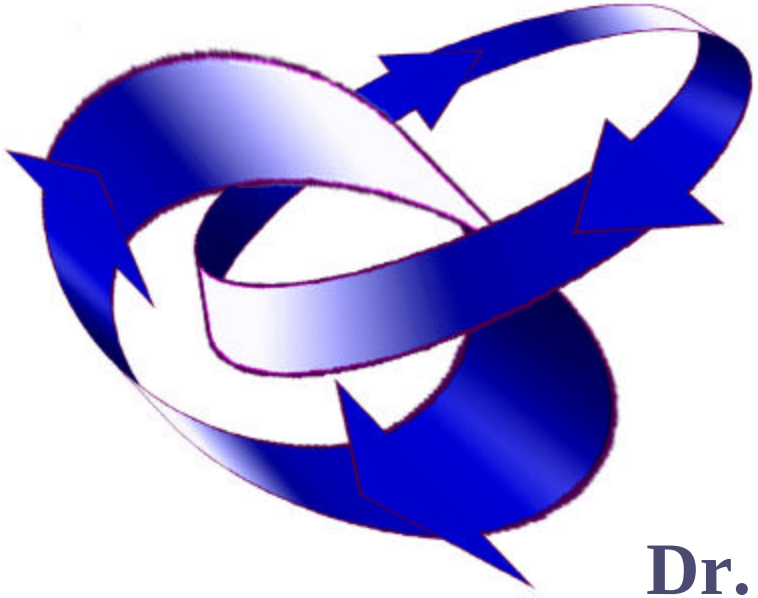
Supporting Science at NIST...



Scientific Applications and Visualization Group

Dr. Judith E. Devaney
Group Leader

http://www.itl.nist.gov/div895/savg

Central Hardware Facilities:

Compute Resources:

IBM SP2:

- 48 node, 80 CPU and a Scalable POWERparallel Switch, 512MB and 2.5GB temporary disk space/node

Four SGI Origin 2000 machines:

- 8 196 Mhz R10000 CPUs, 8 GB of memory, 120 GB of disk space
- 32 250 Mhz R10000 CPUs, 32 GB of memory, 96 GB of disk space
- 32 300 Mhz R12000 CPUs, 32 GB of memory, 193 GB of disk space
- 32 300 Mhz R12000 CPUs, 32 GB of memory, 193 GB of disk space

One SGI Cluster

- five dual processor R10000 CPUs, with 4 GB of memory

One Linux Clusters

- fourty-eight 500Mhz Pentium IIIs connected by a Fast Ethernet network. Each node has 1 cpu with at least 256MB of RAM and 6GB of local disk storage.

Visualization Resources:

- One SGI Onyx with three graphics pipelines, twelve R12K CPUs, 7 GB of memory
- One Wall immersive environment with Crystal Eyes software/hardware with head tracking

Staying Ahead

Parallel Computing

Visualization

Informatics

Science

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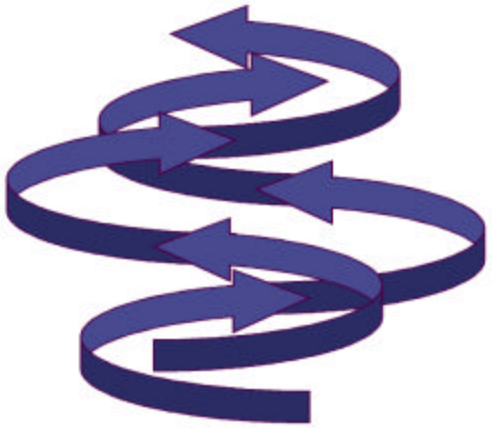
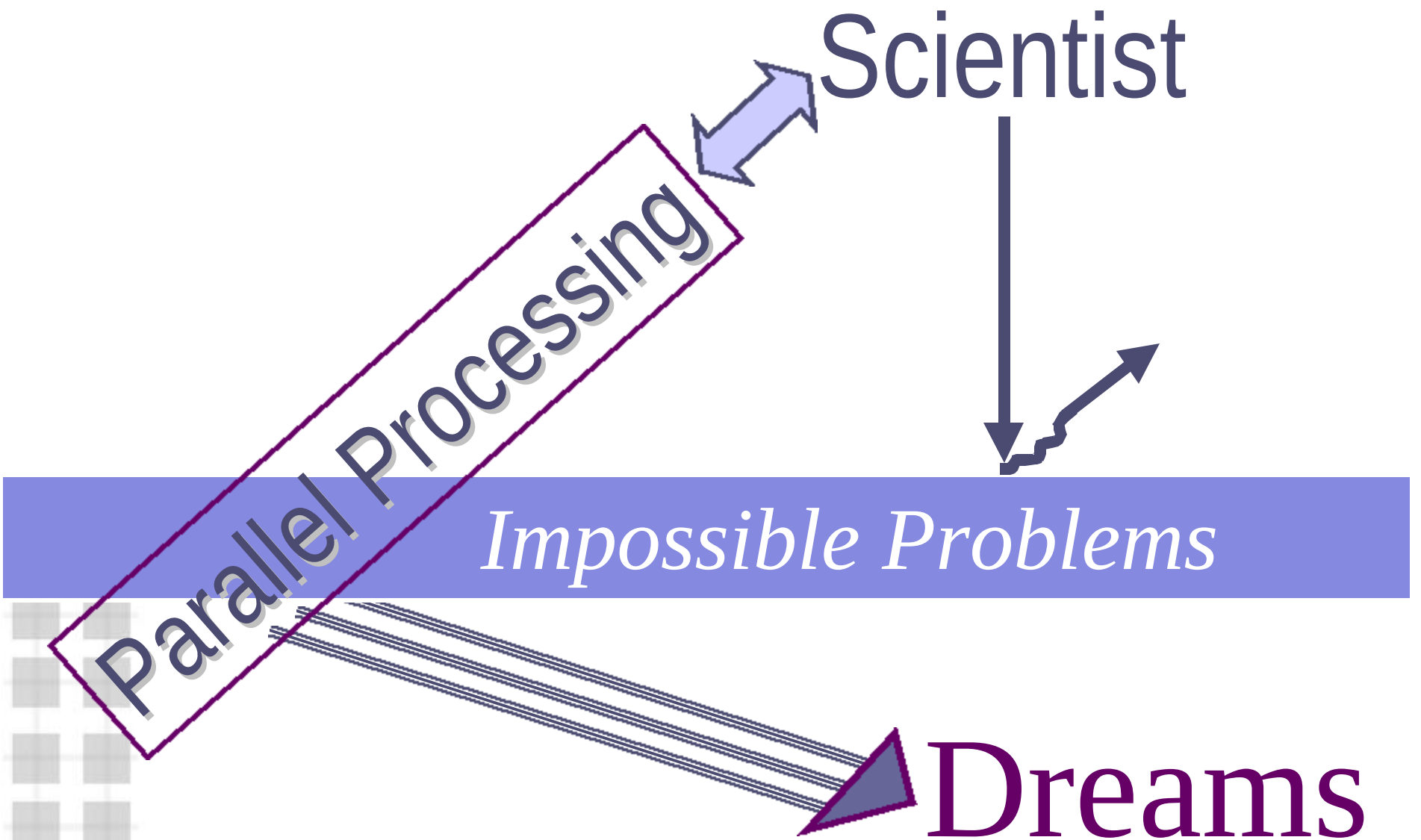
Computing ⇐ *Parallel Processing*

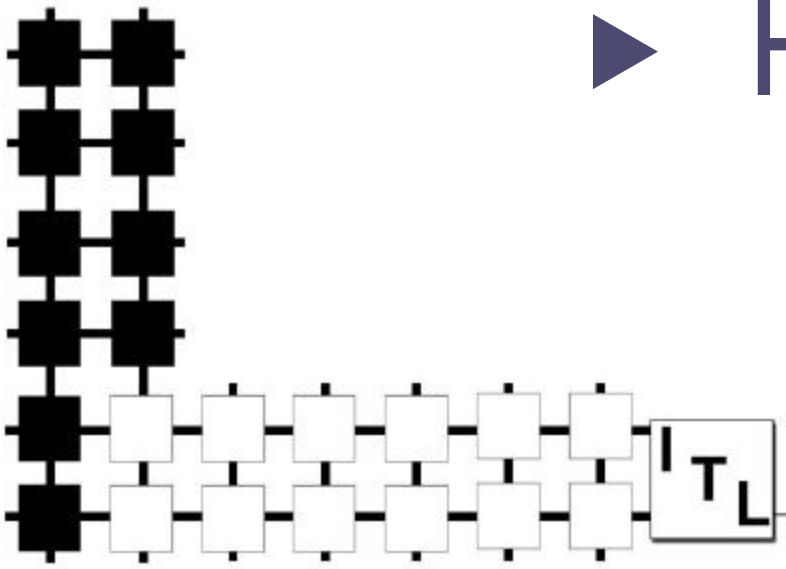


Staying Ahead


Scientist
Parallel Processing
Impossible Problems
Dreams

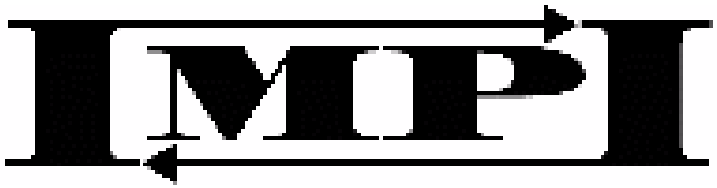
The Role of Standards

- New: MPI
- Future: IMPI



ITL PARALLEL PROCESSING

NIST



Interoperable Message Passing Interface (IMPI)

- Industrial-led effort to create a standard to enable interoperability of different implementations of the Message Passing Interface (MPI).

- Standard vote passed.

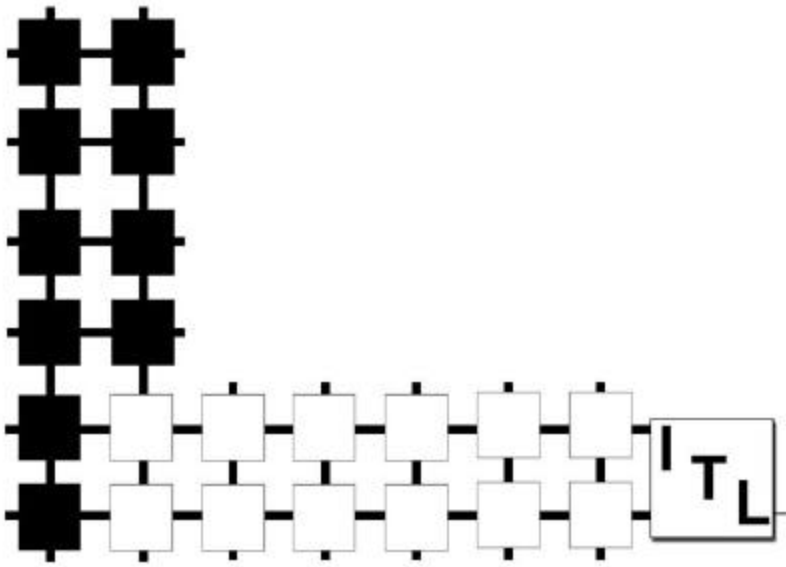
- An IMPI Protocol Conformance Tester has been developed by the NIST/ITL/HPSS/SAVG. It is web based and exercises the whole IMPI Protocol

- LAM 6.4-a2, released November 1999, from the Laboratory for Scientific Computing at the University of Notre Dame supports IMPI. It has passed all NIST tests.

- NIST/ITL/HPSS/SAVG has written an SBIR for the development of an IMPI aware algorithm tuner. It has been awarded to a company that specializes in MPI

New computing environment

- run on everything

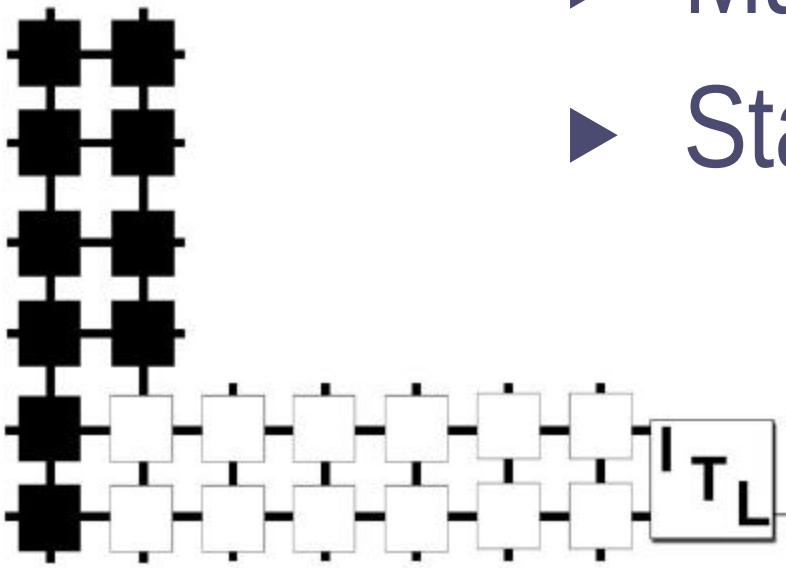


ITL PARALLEL PROCESSING

NIST

Parallel Computing is cross disciplinary:

- Physical scientist
- Computer scientist
- Mathematician
- Statistician

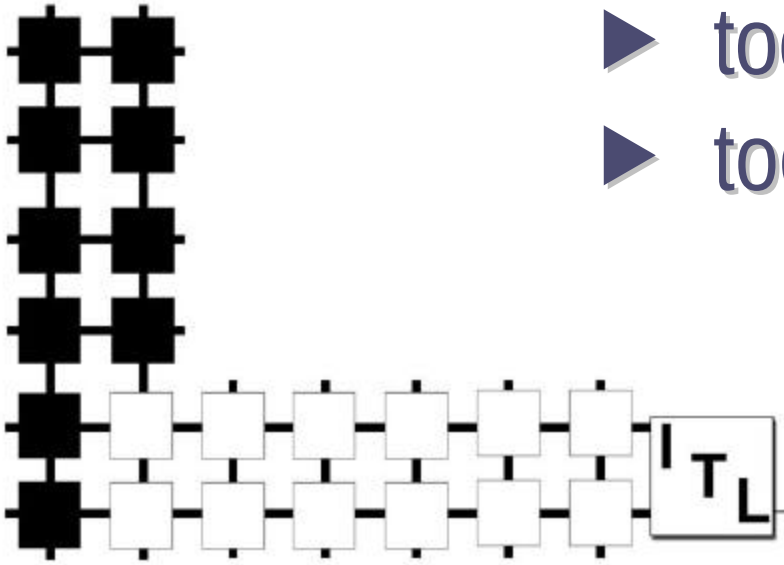


Our Goal:

Help NIST computational scientists advance state of the art in scientists' fields

by doing 'impossible' problems

- too much memory
- too much time
- too many runs



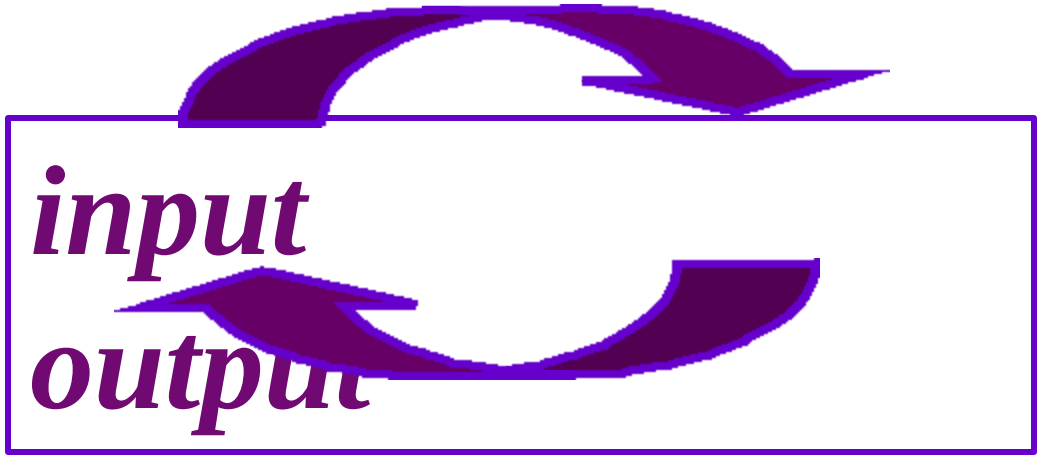
ITL PARALLEL PROCESSING NIST

We supply:

- MPI libraries:
  - DparLib
  - AutoMap/AutoLink
- Parallel Algorithms

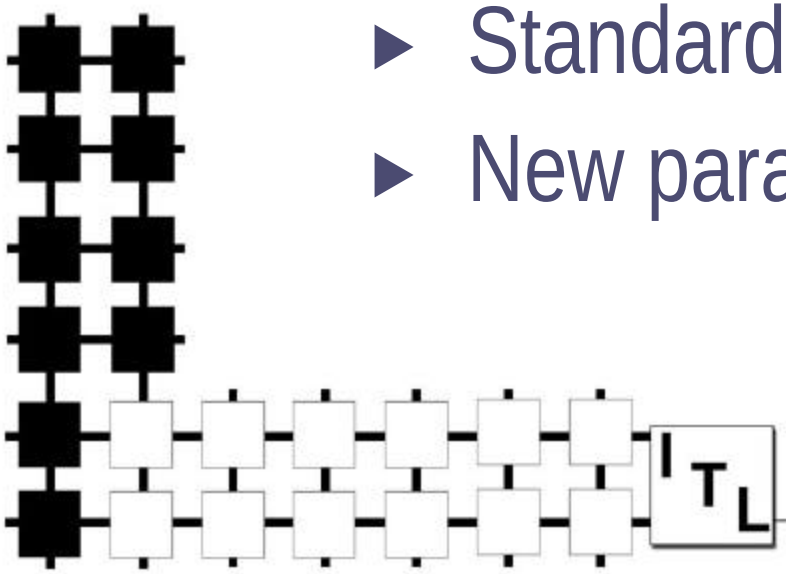
Output:

Portable program driven by input files



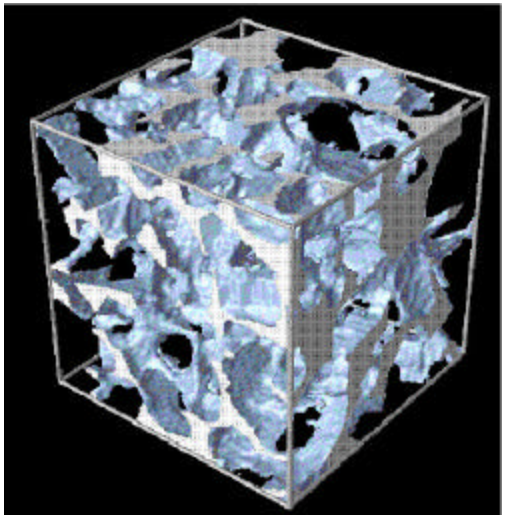
Results:

- Theory validation
- Experiment validation
- New analysis tools
- New insights
- Standard reference codes and data
- New parallel algorithms

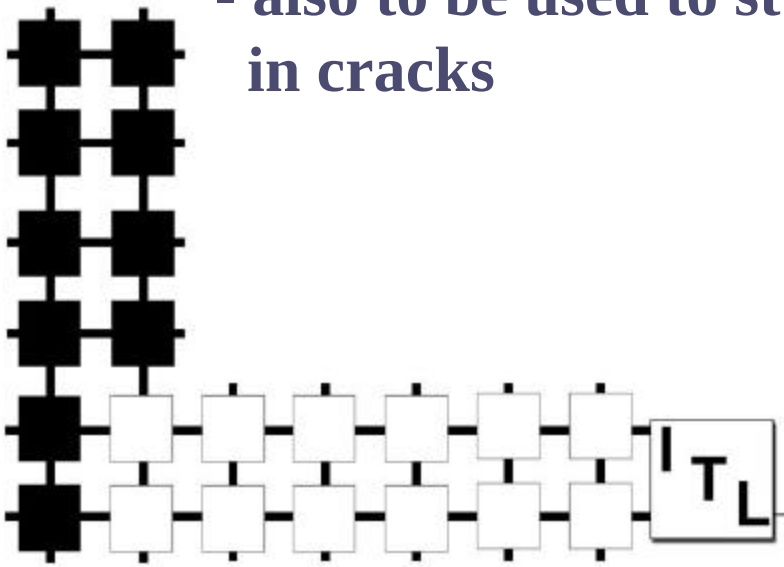


Fluid Flow in Porous Media

Nick Martys BFRL



- state of the art code
- papers, invited book chapter on mesoscale modeling
- now being used by other researchers in BFRL for other work
- also to be used to study flow in cracks



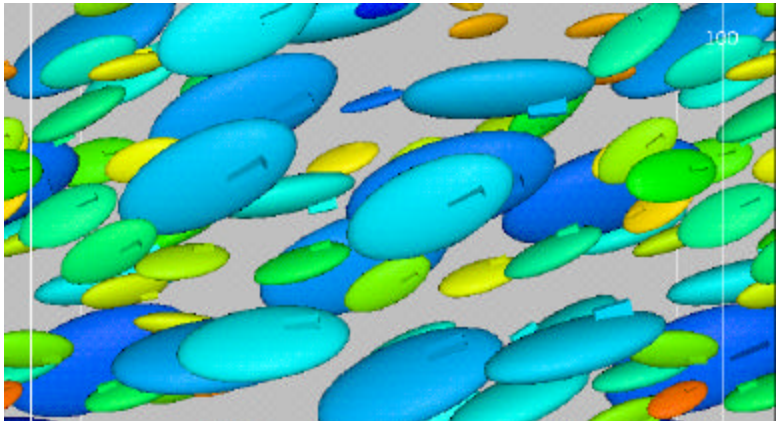
PARALLEL PROCESSING

NIST

Modeling of High Performance Concrete

Nick Martys BFRL

- studying wide range of properties: shape, size distribution, interactions between particles
- comparison with NIST experiments



Science

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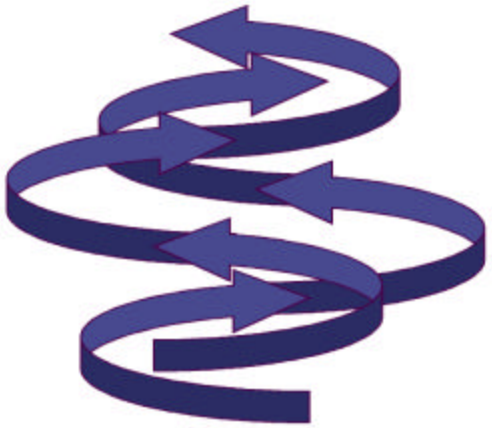
Computing ⇐ *Visualization*

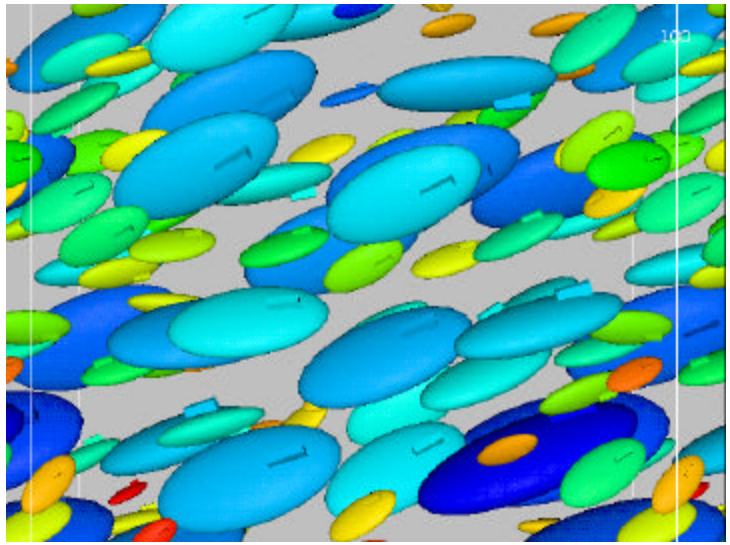


Staying Ahead

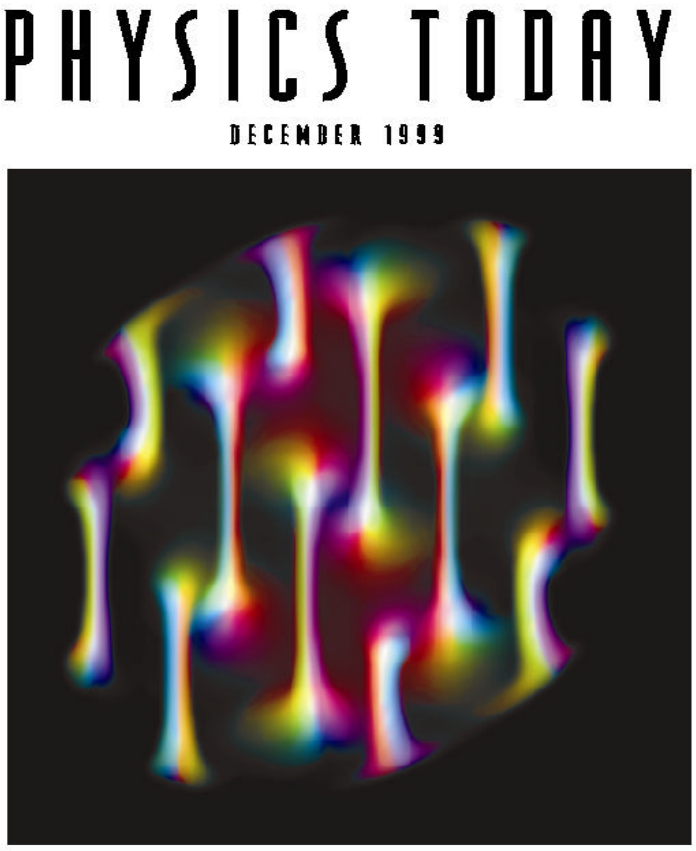
Visualization

Goal: A full immersive environment (CAVE)

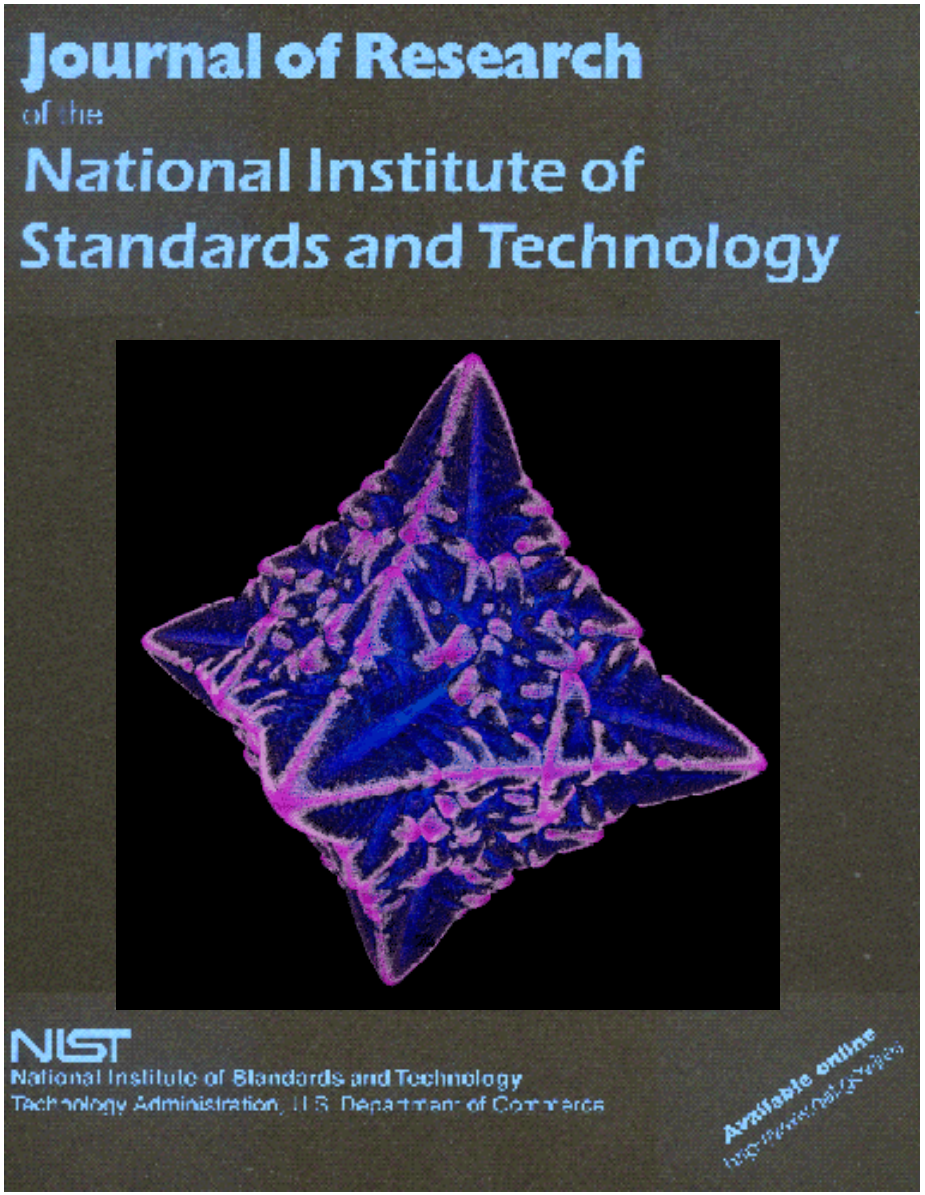
Currently: Stereo capability



Visualization



LOOKING INTO BOSE-EINSTEIN CONDENSATES



Science

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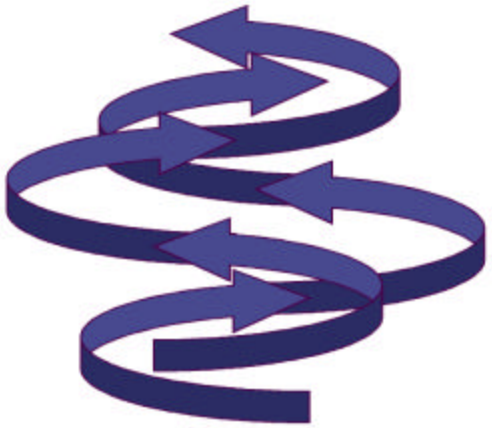
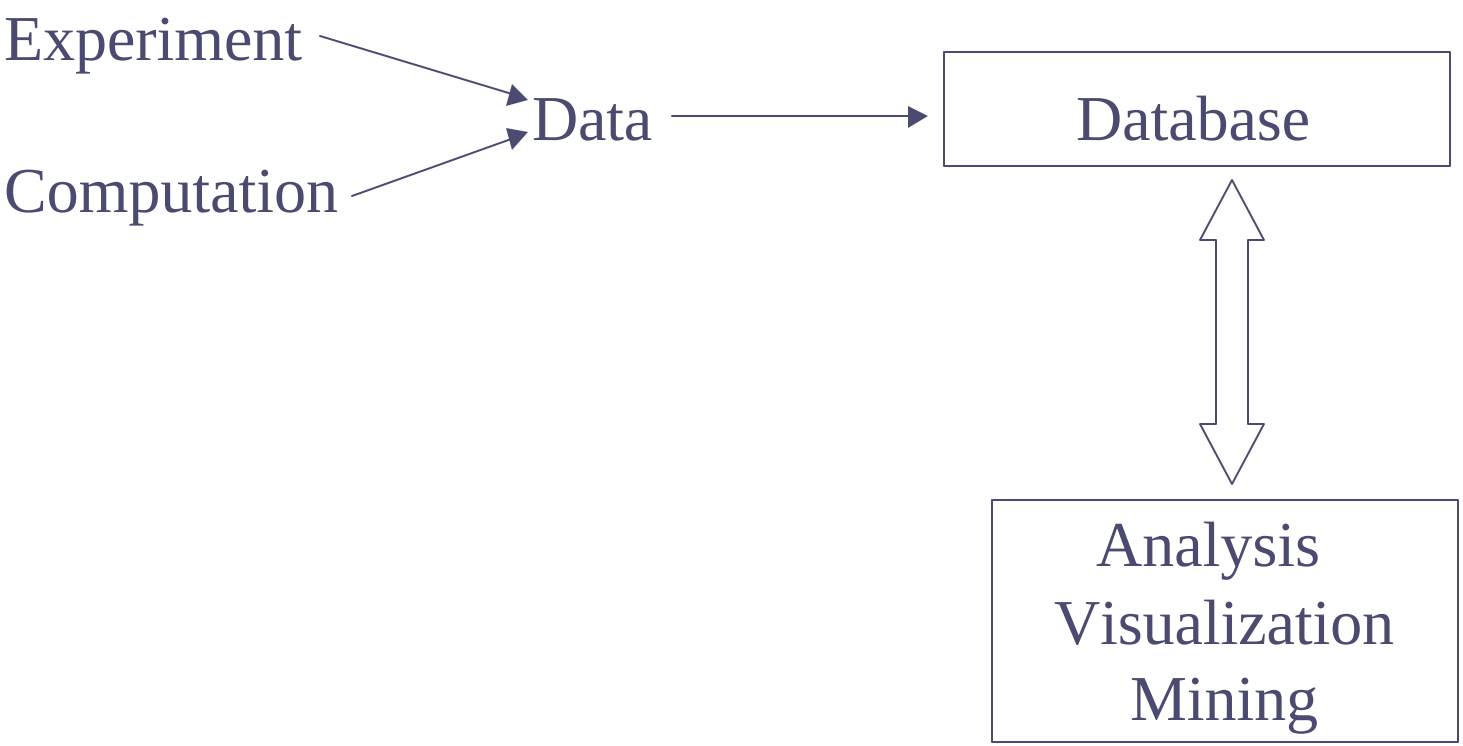
Computing ⇐ *Informatics*

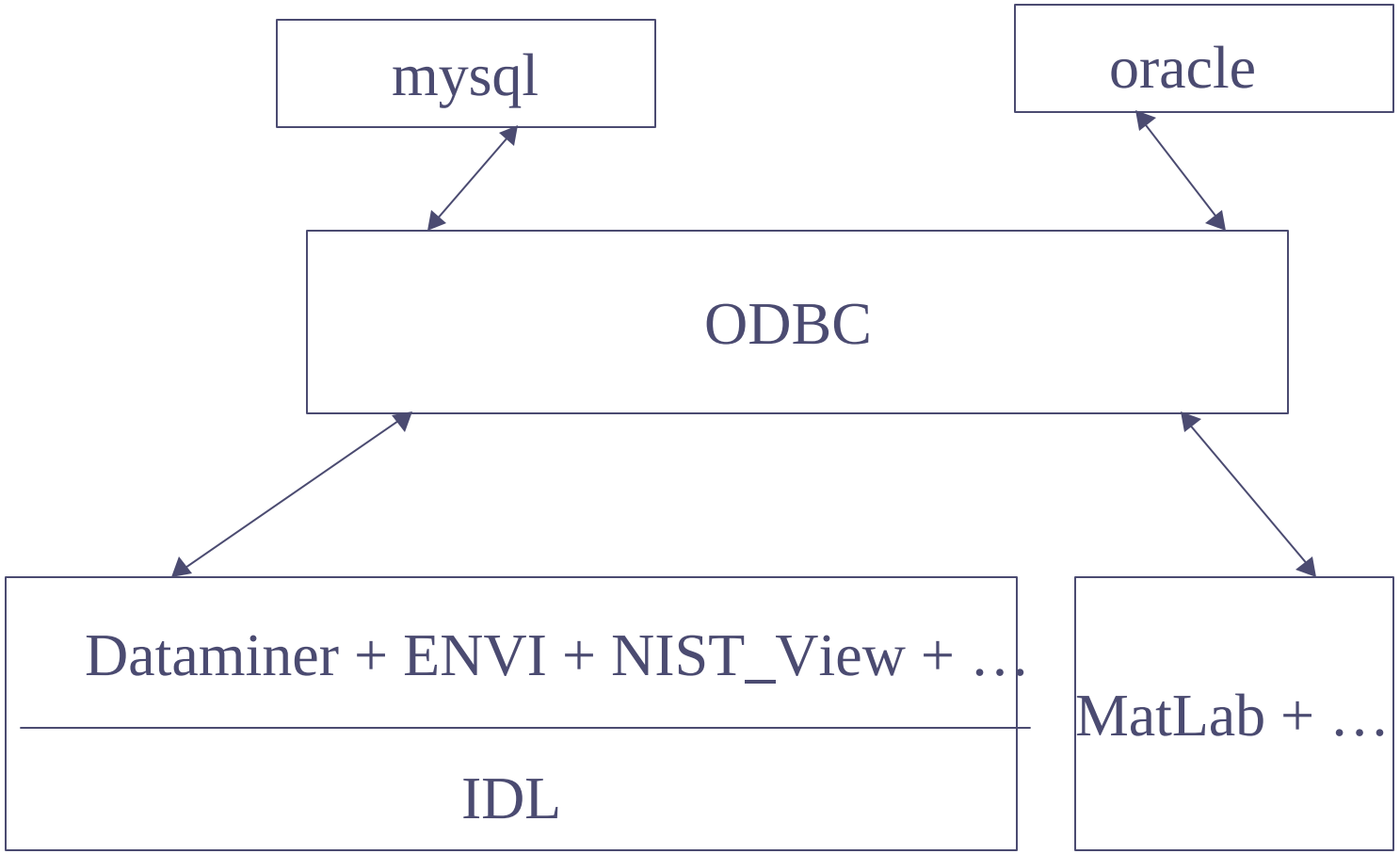


Staying Ahead

Informatics



Informatics

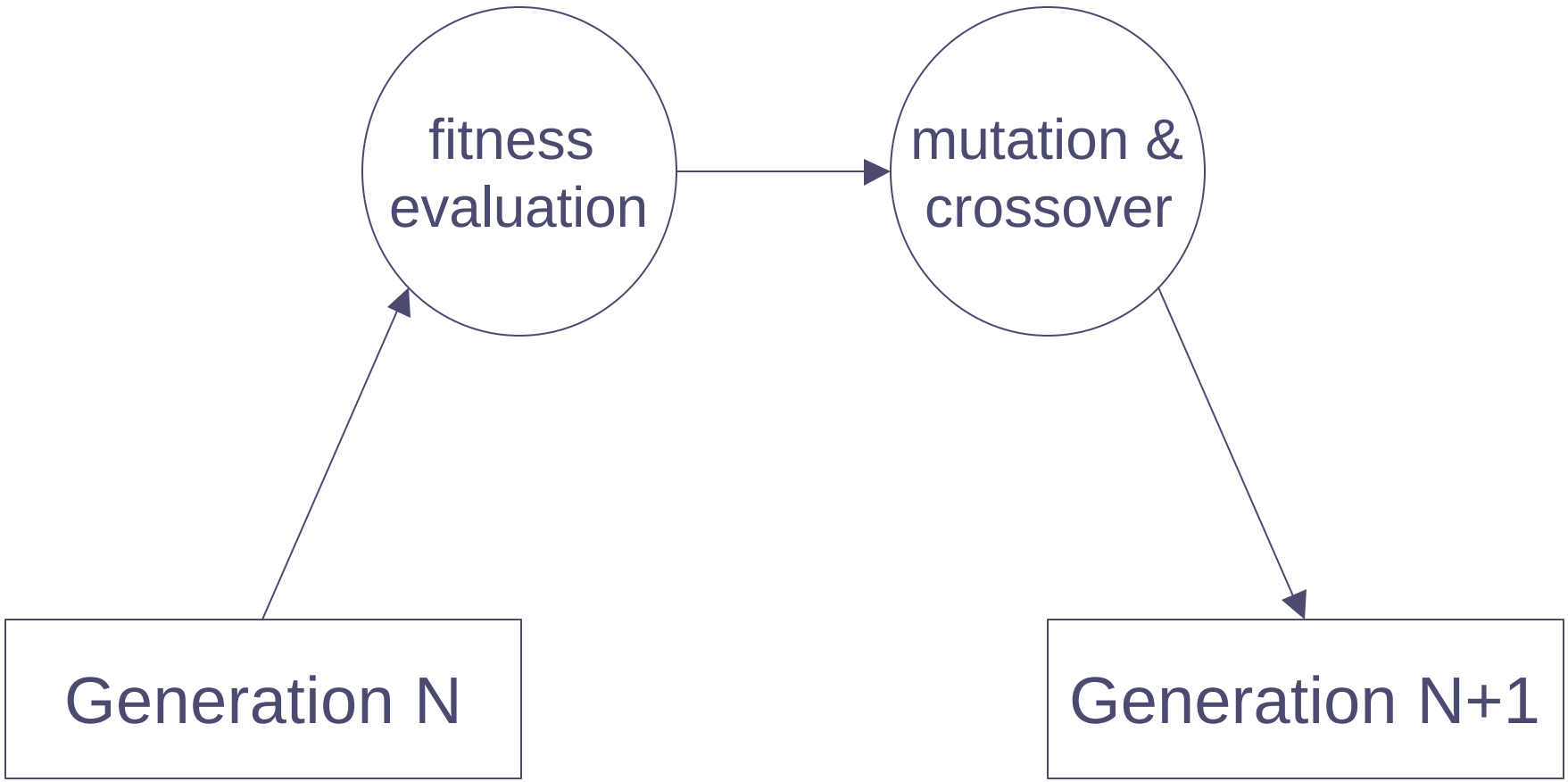


Informatics

Genetic Programming – the evolution of computer programs

- Darwinian selection and reproduction evolve a program that solves a problem.
- Probabilistic techniques generate, combine, and modify a population of programs.
- Problem-specific fitness function determines how well any single program in the population solves the target problem.
- Fitness evaluation drives the evolutions of the population toward a solution.
- GP has been found to be good for function finding and optimization, among other applications.

Evolution of a Generation



The NIST Generic GP System

- Applicable to a variety of problems.
- Accommodates user-supplied operations and fitness functions
- User control of various operating parameters:
  - program structure
  - initialization techniques
  - reproduction strategies
- Parallelization using MPI and AutoMap / AutoLink
- Currently under development

NIST Generic GP System: Applications

- Characterization of measurement errors
- Optimization
  - mixtures
  - Laser parameters
- Data mining algorithms
- Others . . .